MATHEMATICAL MODELLING OF FLUIDIZED BED COAL COMBUSTION

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INTRODUCTION

This report provides an outline of the work done on modelling fluidized bed combustors since July of 1985. As the project is incomplete, this is an interim report.

The report has four sections. The section on the model skeleton is a description of the framework of assumptions used in developing the model. These assumptions range from the division of the combustor into components down to the assumptions necessary to formulate balance equations on each component. The next section presents most of the equations that result and the proposed method of solution. There are a few problematic equations whose formulation remains to be completed. The third section, on the ancillary work, describes various details of the model and the programming. This deals mostly with aspects of the volatile plume phenomenon. The final section summarizes future work required to complete and extend the model.

MODEL SKELETON

The model skeleton is the structure formed by the subdivision of the system into components and the balance of mass and thermal energy on each of the components. No consideration is given at this point to the estimation of parameters or to the form of specific processes.

The model divides the combustor into four components:

- the dense bed
- the splash zone
- the freeboard
- the recycle loop

The dense bed is the region above the distributor plate with a large average volume fraction of particles, having small relative change with height. The extent of this region is determined by operating conditions. The splash zone is a region of transition between the dense bed and the freeboard, characterised by a rapid decrease in particle volume fraction. Under certain operating conditions the splash zone may be negligible, but it is always present in a fluidized bed combustor. The freeboard is the region between the splash zone and the gas exit characterised by a small particle volume fraction, typically less than 0.02. Conditions in the freeboard determine the particle flux recycled to the bed. The recycle loop is the capture of elutriated particles, usually by a cyclone, and the return of a fraction of the captured particles to the bed.

The remainder of this section outlines the modelling assumptions for each component and the next section provides the equations that obtain from such assumptions.

Dense Bed

There are two possible regimes of operation for the bed, namely bubbling and turbulent churning. The bubbling regime is characterised by distinct voids rising through suspended solids and is modelled according to the two-phase analogy. The bubbles are assumed to be free of particles and the suspended particles and associated gas stream are at the conditions of minimum fluidization.[1] The bubble wakes are insignificant or very unstable. The gas velocity in the suspension is greater than the bubble rise velocity, thus the gas streamlines through the bubble are open. These are commonly called slow bubbles, though the name open bubbles is preferred. The turbulent regime has no distinct voids and is assumed to be uniform over a cross-section. In both regimes, total voidage $\bar{\varepsilon}$ is a well defined concept, meaning the fraction of the cross-sectional area occupied by gas. The bubbling regime can be further described by the concepts of emulsion voidage ε_e and bubble fraction δ. The extent of the dense bed is determined from an expression for total voidage and the solids inventory. The total voidage is assumed uniform over the dense bed region.

In both regimes the gas is in plug flow, in one phase when turbulent, in two phases when bubbling. The solids have uniform composition throughout the bed. The bed is isothermal,

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1 At significant bubble fractions the emulsion velocity is probably substantially higher than at minimum fluidization, making a one-phase model more attractive. See A.E. Almstedt [1987] Chemical Engineering Science vol.42, p.581

excepting the small concentration of char particles. The composition of gas is uniform in a phase across a section of the bed. A plume can be incorporated by dividing the cross-section into plume and non-plume areas, with differing uniform gas compositions, and this division must be recognised in the particle reaction calculations. It is further assumed that there is negligible volume change of solids, over the whole bed, due to chemical reaction.

Splash Zone

The extent of the splash zone is determined by the size of bubbles bursting at the top of the dense bed, the superficial velocity, and the particle size distribution. The total voidage increases continuously from the value in the bed to the minimum value for particle transport without choking. The gas-particle mixture is uniform for a cross-section, and the splash zone is well-mixed for both gas and particles. The splash zone is isothermal, though not necessarily at the same temperature as the dense bed, excepting again the char particles. The influx and efflux of gas is determined by conservation of mass, while the particle fluxes are more difficult to model. The particle residence times should be small so the influxes and effluxes to the bed should be large, while the influxes and effluxes to the freeboard are determined by the structure of the gas flow.

Freeboard

The freeboard extends from the top of the splash zone to the combustor exit. There are three phases: gas, rising particles, and falling particles; and each is in plug flow. The particles move at a single velocity in each size fraction and direction, and the transfer between particle phases is only from the rising phase to the falling phase. There is a vertical temperature variation for both gas and particles, with all particles of the same type at the same temperature at a given vertical position. Gas and particle temperatures may be different, cooling walls and radiation from the bed must be considered in the heat balance.

Recycle Loop

The cyclone collects with a general efficiency η for all size fractions, of which a fraction λ is recycled to the dense bed. No flue gas is recycled.

Modes

There is a variety of modes of operation for a model program, depending on which of the operating conditions are regarded as independent or dependent variables. The mode selected here for programming regards the bed temperature, fuel feedrate, and excess air as independent and determines the required cooling heat flux to close the thermal energy balance. This is the simplest mode as it avoids solving the energy balance, and eliminates the dependence on the empirical heat transfer coefficients. This mode also allows the user and programmer to concentrate on the mechanical and chemical processes in the combustor. Furthermore, with the inclusion of a description of the cooling surfaces in the bed and a set cooling load, a non-linear equation solving algorithm can be used with the model to solve for any of the bed temperature, fuel feedrate or fluidizing velocity. Thus this mode can be extended to cover a large number of uses.

EQUATIONS

Gas Balances

For a turbulent bed, the single phase mass balance for species A gives

$$\frac{dc_A}{dz} = \frac{1}{\rho U}\left[(1-\bar{\epsilon})\left(\sigma_A - c_A\sum_B \sigma_B\right) - \bar{\epsilon} r_A\right]$$

where σ_A is the heterogeneous reaction term and r_A is the homogeneous reaction term. The total mass balance, summing over all species, is

$$\frac{d}{dz}(\rho U) = (1-\bar{\epsilon})\sum_B \sigma_B.$$

Thus, for N species, there are N-1 equations to be solved. Since the total gas density is given by

$$\rho = \frac{P}{RT}\left[\sum_B \frac{c_B}{M_B}\right]^{-1}$$

for ideal gases, the superficial velocity is also known. The initial conditions follow immediately from the inlet gas conditions, neglecting the heating time at the distributor plate.

For a bubbling bed, the mass balances on each phase for species A give the equations

$$\frac{dc_A^{(b)}}{dz} = \frac{1}{\rho^{(b)} V_b U_b}\left[r_A(\mathbf{b}) V_b - K S_b\left(\rho^{(e)} c_A^{(e)} - \rho^{(b)} c_A^{(b)}\right) - (1-\bar{\epsilon})\rho^{(e)}\left(\frac{RT}{P m^{(e)}}\right)\sum_B \frac{\sigma_B(\mathbf{e})}{M_B} - c_A^{(b)} U_b \frac{d}{dz}(\rho^{(b)} V_b)\right]$$

for the bubble phase, and

$$\frac{dc_A^{(e)}}{dz} = \frac{1}{\rho^{(e)} U_{mb}}\left[(1-\epsilon)\sigma_A(\mathbf{e}) - \epsilon r_A(\mathbf{e}) - U_{mb} c_A^{(e)} \frac{d\rho^{(e)}}{dz} + \frac{\delta}{(1-\delta)}\left(r_A(\mathbf{b}) - \frac{d}{dz}(\rho^{(b)} U_b c_A^{(b)})\right)\right]$$

for the emulsion phase. The bold-face arguments indicate the phase for evaluation of the reaction term. On the right hand side of the bubble phase equation, the second term gives the interphase transfer, the third term is the saturation flux, and the fourth term accounts for density and volume changes. The emulsion phase equation comes from a balance on the whole bed, the last two terms coming from the bubble phase balance. The first three terms on the right hand side are the heterogeneous and homogeneous reactions and the density change, respectively. The bubble properties V_b, S_b, U_b, and U_{mb}, are known functions of vertical position and the bubbles are assumed to be well-mixed. The initial split of the gas velocity is given by

$$U_b = \frac{U_0 - (1-\delta)U_{mb}}{\delta}$$

and this is used to determine γ in the relationship between bubble size and velocity:

$$U_b = \gamma(U_0 - U_{mb}) + 0.71\sqrt{gD_b}\,.$$

The same reaction routines for r_A and σ_A are used in both sets of equations, one- and two-phase.

The splash zone is well-mixed, so the specific mass balance is

$$c_{A0}I + [\epsilon r_A + (1-\epsilon)\sigma_A]V_{SZ} = c_A E$$

with I being the mass influx and E being the mass efflux. Summing over A determines E,

$$E = I - (1-\epsilon)\sum_B \sigma_B.$$

The average voidage in the splash zone, extending from z_1 to z_2, is

$$\epsilon = \frac{\int_{z_1}^{z_2} \epsilon\, dz}{z_2 - z_1}.$$

In the freeboard, the gas is in plug flow and particle volume fraction α is negligible. The mass and thermal energy balances are linked by the perfect gas equation of state.

$$\frac{d}{dz}(c_A \rho U) = r_A + \alpha\sigma_A$$

$$\rho C_p U \frac{dT}{dz} = \frac{d}{dz}\left(k\frac{dT}{dz}\right) - \sum_B h_B r_B + q_p - q_r - \sum_B \alpha\sigma_B \bar{h}_{sB} - q_w$$

Here, C_p is assumed constant, k is the turbulent thermal conductivity, the q's indicate the gas-particle convective transfer, radiation to the gas, and cooling wall loss, respectively. The summations are the contributions from homogeneous and heterogeneous reactions.

Particle Balances

Particle size distribution is important for reaction modelling, and this is determined by a discretized population balance for a well-mixed vessel. For char, the in-bed equations are

$$-f_i - \Delta\frac{m_i\omega_i}{\Delta d_i} = I_{SZi} + \lambda\eta F_{ei} - E_{SZ}c_i - \frac{Q}{M}m_i - \bar{\Phi}_i m_i - \sum_{k=i-1}^{N} \Delta d_k \overline{(\Phi\omega_i)}_k m_k - \omega_{i1}\sum_{k=2}^{N} m_k \bar{A}_k$$

assuming uniform distribution over a size interval Δd_i, no density change, no fracture products within the source particle size interval, and all attrition products in the smallest size interval. The various terms are as follows :

f_i is the feedrate in size interval i,

$\Delta\frac{m_i\omega_i}{\Delta d_i}$ is the rate of mass loss by continuous processes, combustion and attrition,

I_{SZi} is the influx of particles from the splash zone,

$\lambda\eta F_{ei}$ is the recycle rate term, with F_{ei} being the particle flux out of the freeboard,

E_{SZ} is the efflux to the splash zone,

$\frac{Q}{M}m_i$ is the bed product extraction rate, with M the total mass of particles in the bed,

$\bar{\Phi}_i m_i$ is the mass loss by fracture,

$\Delta d_k \overline{(\Phi\omega_i)}_k m_k$ is the mass gained from fracture of larger particles,

$m_k\bar{A}_k$ is the mass gained from attrition during combustion.

For stone, meaning a sorbent like limestone or an inert like sand, the in-bed equations are

$$\frac{dm_i}{d\theta} = \overline{\left(\frac{\nu_p}{\nu_p}\right)}_i m_i + I_{SZi} + \lambda\eta F_{ei} - E_{SZi} - \frac{Q}{M} m_i$$

where θ is the residence time and the first term on the right hand side is the rate of density change, assuming no size change. The feedrate is the initial condition for this system of equations.

For the splash zone, fracture and attrition are neglected for char, and all other bed assumptions are retained. The equations are

$$\Delta\frac{m_{i,out}}{\Delta d_i} = I_{BEDi} - E_{BEDi} + I_{Fi} - E_{Fi}$$

$$\frac{dm_i}{d\theta} = \overline{\left(\frac{\nu_p}{\nu_p}\right)}_i m_i - I_{BEDi} - E_{BEDi} - I_{Fi} - E_{Fi}$$

The two particle phases in the freeboard are in plug flow. The discretized population balance equations are

$$\frac{d}{dz}(m_{ut,out}\overline{v_{put}}) + \Delta\frac{m_{ut,out}}{\Delta d_i} = -\bar{S}_i$$

$$\frac{d}{dz}(m_{di,out}\overline{v_{pdi}}) + \Delta\frac{m_{di,out}}{\Delta d_i} = \bar{S}_i$$

for char, and

$$\frac{d}{dz}(m_{ut,out}\overline{v_{put}}) = -\bar{S}_i$$

$$\frac{d}{dz}(m_{di,out}\overline{v_{pdi}}) = \bar{S}_i$$

for stone, neglecting reaction. The velocities v and transfer functions $\bar{S}_i$ are determined partially by the gas properties, so gas and particle freeboard equations are all coupled.

It is appropriate at this point to discuss how the equations are to be handled and what methods will be used to produce approximate solutions. The equations are coupled among all four of the components of the combustor for the particles, so the particle balance equations must be solved simultaneously. The gas balance equations could be solved sequentially, but these are coupled with the particle equations, especially in the freeboard. A simultaneous solution of the gas and particle equations is not feasible because of the mixture of plug flow and well-mixed models in the dense bed region, and so an iterative solution must be tried. The solution procedure will have the following general form:

estimate bed hydrodynamics and define extent of dense bed, splash zone and freeboard
make initial estimate of gas concentrations over whole combustor
iterate
    solve particle balances over dense bed and splash zone
    solve gas balances over dense bed and splash zone
    solve gas and particle freeboard balances simultaneously
until solutions converge

The systems of differential equations for gas balances and particle balances in the freeboard are solved by numerical integration using a fifth order Runge-Kutta, or Gear's method if necessary. The char particle population balances are linear algebraic equations and are solved using the standard Gaussian elimination methods. The residence time distributions for stone in the bed and splash zone are estimated analytically.

ANCILLARY WORK

Plume Calculations

The work done on the plume submodel can be divided into three areas, namely the gas dispersion from a distributed source of volatiles, the motion of particles over small times after being fed to the bed, and the comparison of time scales of the relevant processes.

Time Scales

There are four processes which are relevant to the plume model: the transport of volatiles through the bed; the convective or dispersive transport of particles in the bed; the rate of volatiles release from the coal particles; and the feedrate of large coal particles. The gas has been assumed to be in plug flow (in both turbulent and bubbling regimes), so the residence time of volatiles is

$$\tau_g = \frac{H}{U}$$

For a turbulent bed U is the superficial gas velocity, but in the bubbling regime it is a composite of bubble and emulsion velocities. The particles can be assumed to be convected at some mean velocity as a result of the circulation induced by the gas flow. This velocity will depend on the location of the feed point and the geometry of the bed, the usual pattern being downflow along the walls and upflow in the centre. The rise time is an important parameter since at the top of the bed the particles enter the splash zone or become mixed in the bed. Assuming a central feed point at the bottom of the bed, and the mean velocity being U_p, the particle rise time is

$$\tau_{pr} = \frac{H}{U_p}.$$

The devolatilization time of large coal particles, τ_v, is usually given by a power law correlation with the particle diameter, the exponent taking a value between 1 and 2. For a 20 mm particle all the volatiles are released after 200 seconds. When the fuel is composed of large lumps and the feedrate is low, it is possible that the time between the feeding of individual lumps is comparable with the other time scales. The time between lumps entering the bed is given by

$$\tau_{fp} = \frac{\frac{\pi}{6}\rho_p d_p^3}{F_c}$$

Discrete plumes, each particle producing a separate plume, would result when τ_v and τ_{fp} are comparable, but for coal particles 20 mm in diameter and at a feedrate of 15 kg/m^{2}h τ_{fp} is about 5 seconds, much smaller than the devolatilization time. The other condition for a discrete plume model is that the particle rise time is smaller than the feed time. The mean particle velocity is difficult to measure, but recent papers give velocities which produce rise times in the range from 5 to 20 seconds.[2] Thus a continuous feed can be assumed, except in certain pathological situations.

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2 G.M. Rios, K. Dang Tran, H. Masson [1986] "Free Object Motion in a Gas Fluidized Bed" Chemical Engineering Communications vol.47,pp.247-272
S. Yoshioka et al. [1987] "Circulatory flow of particles in a 0.96-m-diameter fluidized bed" International Chemical Engineering vol.27, pp.281-287

Gas Dispersion in Plug Flow

The equation for convective dispersion of a gas with a distributed source and no reaction is

$$U\frac{\partial c}{\partial z} = D_r\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) + D_a\frac{\partial^2 c}{\partial x^2} + \Sigma$$

This equation has been solved for a rectangular bed with impermeable walls, assuming the source term has a double finite Fourier transform. No reaction is included in this equation, but by assuming that the volatiles concentration is a negative oxygen concentration, a subtraction will give an approximation to the plume region. This can be used in a one-dimensional bed model as indicated in an earlier section. The solution depends strongly on the magnitude of the source term, which in turn depends on the particle motion a short time after feeding. The problem of particle motion is discussed in the next section.

Particle Circulation

Circulation of particles exists in fluidized beds, even in particulate fluidization. This casts doubt on successful modelling of small time particle motion by a simple dispersion coefficient, which neglects this circulation. Soo[3] presented equations for the flow of gas and particles in a particulately fluidized bed, and gave an approximate solution for two-dimensional beds. Exact closed form solutions for the two-dimensional and cylindrical bed geometries have been found. These equations can be modified to incorporate the effect of bubbles and solved to estimate the particle motion in a bubbling bed.

Gas Property Estimates

The FBC model requires values for the specific heat, entropy, and enthalpy of the components of the gas in the combustor. The JANAF values for the species under consideration over the range from 300 K to 1300 K have been fitted with least-squares polynomials of order from 0 to 5. The polynomial of smallest order with error less than 1% at each data point was selected. The values were plotted over the full range as a check for oscillations, and none were found.

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3 S.L. Soo [1986] "Note on Motions of Phases in a Fluidized Bed" Powder Technology vol.45, pp.169-172

FUTURE WORK

The model skeleton needs a musculature of submodels to be a useful tool. Many of these are available from Preto's model,[2] so the following projects will complete the musculature and the model.

Attrition and fragmentation models are needed for the char particle balance equations in the dense bed. For plume calculations, small-time solutions for particle motion are needed. The reactions within the plume, especially lime with H_2S, have to be modelled.

The splash zone is a transition region which is defined by the particle influxes and effluxes. The influx from the bed is produced by the bursting bubbles and a critical evaluation of the available models will be performed. The efflux to the freeboard will be based on a choking criterion similar to Matsen's,[3] which requires an improved slip velocity - voidage relationship. A voidage profile must be assumed or obtained from the literature.

The transfer relation from up-flowing to down-flowing particles in the freeboard must be determined. This is expected to depend partially on the vertical and lateral temperature profiles, so the effect of radiation from the bed and radiation to the walls will be calculated.

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2 F. Preto [1986] "Studies and Modelling of Atmospheric Fluidized Bed Combustion of Coal" Doctoral Thesis, Queen's University, Kingston

3 J.M. Matsen [1982] "Mechanisms of Choking and Entrainment" Powder Technology, vol.32, pp.21-33

NOMENCLATURE

Subscripts

A, B	chemical species
BED, F, SZ	labels for fluxes to and from the dense bed, freeboard, splash zone
i, k	indices for size intervals in particle population balance
p	particle property
u, d	freeboard particle phase, up and down respectively
0	at inlet or feed conditions

Superscripts

(e)	in the emulsion phase
(b)	in the bubble phase

Latin

A	mass rate of generation of fines by attrition per unit mass of source particles, s^{-1}
c	mass fraction of a gaseous species
C_p	specific heat at constant pressure, J/kg K
d	particle diameter, m
D_a	axial dispersion coefficient of gas in the dense bed, m^2 /s
D_b	equivalent volume diameter of a single bubble, m
D_r	radial dispersion coefficient of gas in the dense bed, m^2 /s
E	mass efflux term for well-mixed balance equations, kg/s
F_c	mass feedrate of fuel to the bed, kg/s
F_e	mass flux of particles from the freeboard, kg/s
g	acceleration due to gravity, m/s^2

h	enthalpy of reaction for homogeneous reaction, J/kg
$\bar{h}_s$	enthalpy of reaction for heterogeneous reaction, J/kg
H	expanded bed height, m
I	mass influx term for well-mixed balance equations, kg/s
k	turbulent thermal conductivity of gas in freeboard, J m^2/s K
K	interphase mass transfer coefficient in dense bed, m/s
m	mass of particles on a size interval, kg
M	total mass of particles in the dense bed, kg
M_B	molecular mass of chemical species B, kg/mol
n	total molar density of gas, mol/m^3
P	gas pressure in combustor, Pa
q_F	heat flux from particles to gas by convection, J/m^3 s
q_r	heat flux to gas by radiation from bed and particles, J/m^3 s
q_w	heat flux from gas to cooling surfaces, J/m^3 s
Q	mass flow rate of solids from bed by extraction, kg/s
r	rate of homogeneous reaction per unit volume of gas, kg/m^3 s
R	gas constant, J/mol K
S	mass transfer rate from rising particle stream to falling particle stream, kg/s
S_b	surface area of a single bubble, m^2
T	absolute temperature, K
U	superficial gas velocity, m/s
U_b	visible bubble velocity, m/s
U_{mb}	superficial velocity at minimum bubbling (minimum fluidization), m/s
v_p	particle velocity in freeboard, m/s
V_b	volume of single bubble, m^3
x, y, z	Cartesian coordinates in combustor, m

Greek

α	volume fraction of particles in freeboard
β	bubble volume fraction in dense bed under two-phase analogy
γ	coefficient of adjustment for bubble velocity correlation
δ	Kronecker delta symbol
ϵ	emulsion voidage under two-phase analogy
$\bar{\epsilon}$	total voidage
$\hat{\epsilon}$	average voidage in splash zone
η	general collection efficiency of cyclone
θ	residence time of stone particles, s
λ	mass fraction of cyclone product recycled
ρ	mass density of gas, kg/m^3
ρ_p	average mass density of a particle, kg/m^3
$\dot{\rho}_p$	rate of change of average mass density of particle, kg/m^3 s
σ	rate of heterogeneous reaction per unit volume of solids, kg/m^3 s
Σ	distributed volatiles source term for plume, s^{-1}
τ_{fp}	time between feeding of large coal particles, s
τ_g	characteristic residence time of gas in dense bed, s
τ_{pr}	characteristic particle rise time in dense bed, s
τ_v	devolatilization time of a coal particle, s
ϕ	size distribution of particles generated by fracture, m^{-1}
Φ	fracture rate per unit mass of source particles, s^{-1}
ω	rate of change of particle size by continuous processes, m/s